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STRUCTURE AND DYNAMICS CARBOHYDRATE-WATER-SALT SOLUTIONS AS DERIVED FROM MOLECULAR DYNAMICS SIMULATIONS

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Aqueous solutions of carbohydrates are frequently used by electrochemists as systems with variable viscosity. At high concentrations these solutions are known to reveal a complex (heterogeneous) structure. On the other hand, an addition of salt makes it possible to measure the electroconductivity of such electrolytes. The diffusion of ionic components in abovementioned systems attracts attention from both theoretical and practical viewpoint, albeit its mechanism is still poorly understood so far. We report here the first results obtained from molecular dynamics (MD) simulations elucidating some microscopic aspects of the diffusion mechanism. Water-glucose-NaCl soultions are addressed as a model system. MD simulations were performed using the program package LAMMPS [1]. We employed the standard SPC/E model for the water molecules and the OPLS-AA [2] force field was used to describe interatomic interactions in carbohydrates. The force field for ions was taken from Ref.[3]. We discuss the diffusion coefficients of glucose and water molecules, as well as of the Na+ and Cl- ions calculated as a function of the glucose concentration varied in a wide range. The computational results are compared with original experimental data. A challenging difference between the behaviour of Na+ and Cl- ions is predicted which stems most likely from the different life times of glucose - Na+ and glucose - Cl- associates. The relaxation times and hydration numbers are calculated as well and compared with available literature data.

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